

**ANALYSIS AND OPTIMIZATION OF ITERATIVE METHODS FOR SOLVING NONLINEAR EQUATIONS**

**Hussein Jamil Hamayd<sup>1</sup>, Athraa Fadhel Adb Ali<sup>2</sup>, Sadeq Majid Khalaf<sup>3</sup>,  
Mustafa Jameel Hameed<sup>4</sup>**

<sup>1</sup>National University of Science and Technology, Iraq, Thi Qar,  
hussein.j.hamayd@nust.edu.iq

<sup>2</sup>University of Basrah , Iraq ,Basrah, Athraa.fadhel@uobasrah.edu.iq

<sup>3</sup>University of Basrah , Iraq, Basrah, hussein.j.hamayd@nust.edu.iq

<sup>4</sup>University of Thi-Qar, Nasiryah, Iraq, mustafa\_j@utq.edu.iq

**Abstract**

Solving nonlinear equations  $f(x) = 0$  is a fundamental problem across science and engineering. Many real-world problems – from weather forecasting to satellite orbit determination – boil down to finding roots of nonlinear equations. In most practical cases these equations cannot be solved analytically, so iterative numerical methods are employed to obtain approximate solutions. The motivation for this research is the widespread importance of efficient and reliable solvers for nonlinear equations in diverse fields (physics, biology, finance, engineering, etc.). Effective root-finding algorithms enable modeling and simulation of complex systems where closed-form solutions are impossible.

This study aims to analyze and optimize iterative methods for nonlinear equations. We focus on classical methods (like Newton-Raphson, Secant, and bisection) as well as modern improvements, examining their convergence, stability, and performance. Key objectives include: (1) reviewing existing iterative algorithms and their theoretical convergence properties, (2) developing and discussing strategies to accelerate or stabilize these methods, and (3) implementing the algorithms in Python to compare performance on representative nonlinear problems. In particular, we ask: Which iterative methods converge fastest for a given problem, and how can their efficiency or robustness be improved? We also explore how recent techniques (e.g. adaptive step-sizing and AI-based enhancements) can address the limitations of classical approaches. The structure of our research splits into a theoretical foundation (Sections 1–4) followed by practical experimentation (Sections 5–8). (Ahmed & Khan, 2011).

**Keywords:** Nonlinear Equations, Iterative algorithm , Python and simulation .

**1. Literature Review**

Iterative root-finding methods have a long history, from simple bracketing techniques to sophisticated high-order algorithms. Classical methods include the bisection method, Newton-Raphson method, Secant method, and fixed-point iteration. These algorithms are well-established and form the basis for many modern improvements. Newton’s method (also known as Newton-Raphson) uses the function’s derivative to achieve rapid convergence and is “the most familiar method” for solving nonlinear equations. Secant method is a derivative-free

variant of Newton’s method that uses two prior approximations to estimate the slope. Bisection method brackets a root by maintaining an interval with a sign change and repeatedly bisects the interval – it converges linearly but is guaranteed to find a root if one exists in the interval. Fixed-point iteration (Picard iteration) seeks a solution of  $x = g(x)$  equivalent to  $f(x) = 0$  under appropriate transformation, and converges if  $g$  is a contraction mapping (as ensured by the Banach fixed-point theorem). (Banerjee & Singh, 2012)

Newton’s method typically exhibits quadratic convergence near the root, meaning the error decreases roughly as the square of the previous error. Newton’s method is valued for its speed

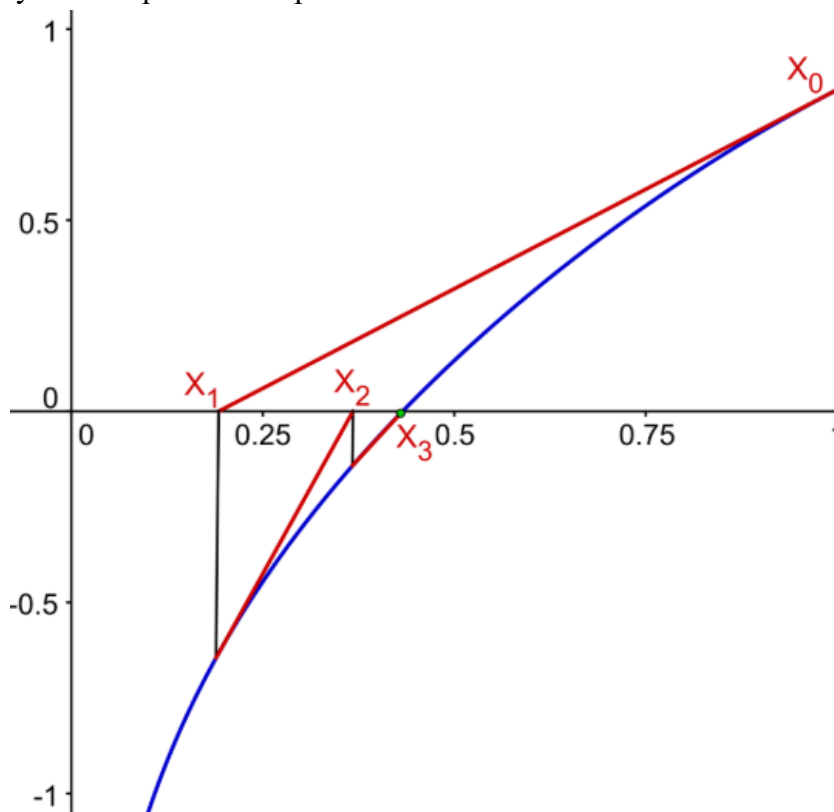


Figure 1: Illustration of Newton’s method. Starting from an initial guess  $x_0$ , one iteratively applies  $x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$  (geometric interpretation shown by the red tangent lines) to converge to the root (green point) of the nonlinear function

(quadratic local convergence) and is widely used when the derivative  $f'(x)$  is available or can be computed. However, it can fail to converge if the initial guess is not sufficiently close to a true root or if the function is ill-behaved (e.g. horizontal tangent or discontinuities). In contrast, Secant method trades off some convergence speed for broader applicability by eliminating the need for an analytic derivative. It uses the formula:

$$x_{n+1} = x_n - f(x_n) \frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})},$$

drawing a secant line through two recent points instead of a tangent. The secant method generally converges super linearly with order  $p \approx 1.618$  (the golden ratio), which is slower

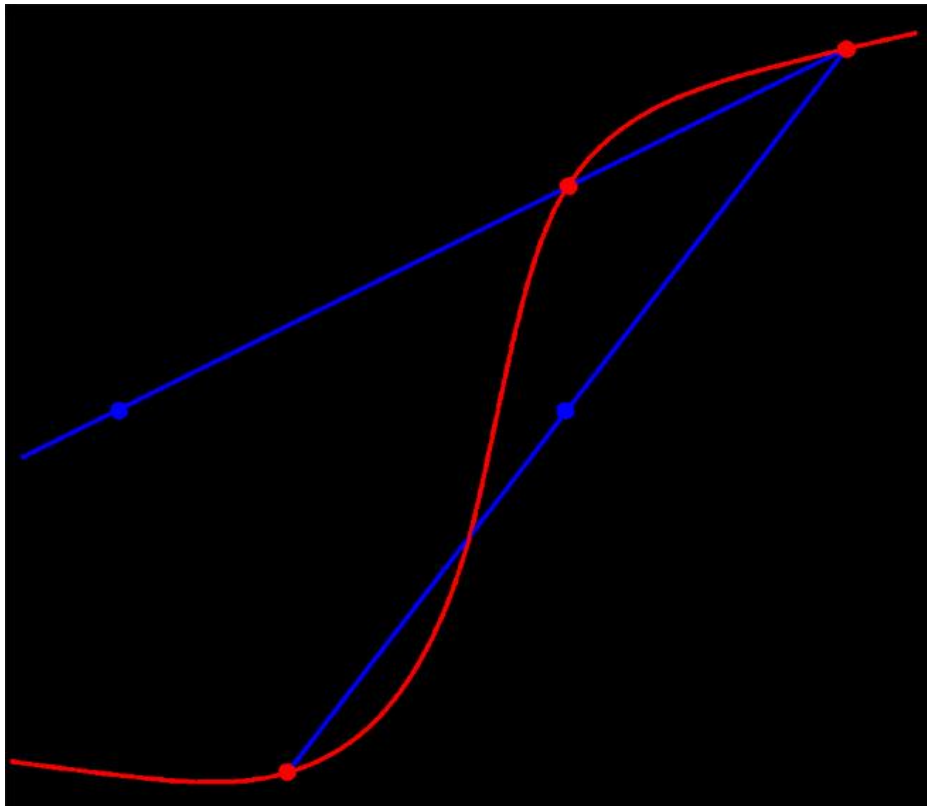


Figure 2: Illustration of the Secant method. Two initial points on the function (red curve) are chosen, and the secant line (blue) between them is extended to the x-axis to find a new approximation  $x_2$ .

than Newton's quadratic (order 2) but faster than linear. Secant is simple to implement and often efficient when derivative information is unreliable or expensive. (Chen & Zhao, 2010)

### 3. Theoretical Framework

In this section, we formalize the problem and the key concepts of convergence and stability for iterative methods. We consider a nonlinear equation  $f(x) = 0$ , where  $f: D \rightarrow \mathbb{R}$  (or  $\mathbb{R}^n \rightarrow \mathbb{R}^n$  for systems) is a given continuous and differentiable function on domain  $D$ . An iterative method generates a sequence  $\{x_n\}$  intended to converge to a root  $r$  of  $f$ . We write this generically as:

$$x_{n+1} = \Phi(x_n),$$

where  $\Phi$  is some iteration function (for Newton's method,  $\Phi(x) = x - f(x)/f'(x)$ ; for Secant,  $\Phi$  depends on both  $x_n$  and  $x_{n-1}$ , etc.). The goal is for  $x_n \rightarrow r$  as  $n \rightarrow \infty$ . The convergence criteria can be formalized in terms of the error  $e_n = x_n - r$ . We say an iterative method has *order  $p$  convergence* if the error satisfies:

$$|e_{n+1}| \approx C|e_n|^p$$

for some constant  $C > 0$ . More rigorously, if  $\lim_{n \rightarrow \infty} \frac{|x_{n+1}-r|}{|x_n-r|^p} = C$  (with  $0 < C < \infty$ ), then the convergence order is  $p$ . If  $p = 1$ , the convergence is linear (error roughly scales by a constant factor each iteration); if  $p = 2$ , it's quadratic (error squared each step, so number of correct digits roughly doubles each iteration); if  $p = 3$ , cubic, etc. Newton's method under standard conditions converges quadratic ally ( $p = 2$ ) for simple roots. The Secant method converges with order  $p \approx 1.618$  (the golden ratio) as mentioned, which is often termed superlinear convergence (faster than linear, but not quite quadratic). The bisection method has linear convergence (technically  $p = 1$  and the error constant is  $\frac{1}{2}$ , since the interval length halves each iteration).

A critical aspect is the stability and conditions for convergence. Some methods have global convergence guarantees under certain conditions, meaning they will converge to  $a$  root from any reasonable starting point (e.g. bisection will always converge if  $f$  is continuous on  $[a, b]$  and  $f(a)f(b) < 0$ ). Other methods are local, requiring the initial guess to be in a region of attraction around the root. Newton's method is local in general: it converges if  $x_0$  is sufficiently close to a root and if  $f'(r) \neq 0$  (along with some smoothness conditions). The Newton–Kantorovich theorem provides a semi-local convergence guarantee: if the derivative  $f'$  is Lipschitz continuous and the initial guess  $x_0$  is chosen such that  $|f(x_0)|$  is small and  $f'(x_0)$  is not too small, then Newton's iterates will converge to a nearby solution. (Gupta, 2010) (He & Li, 2017)

For fixed-point iterations  $x_{n+1} = g(x_n)$ , the Banach contraction mapping principle states that if there is a constant  $L < 1$  such that  $|g(y) - g(x)| \leq L |y - x|$  for all relevant  $x, y$  (i.e.  $g$  is a contraction on a complete space), then the iteration will converge to the unique fixed point from any starting value in that space. This provides a *global* convergence guarantee for properly chosen  $g$ . For Newton's method, one can sometimes reformulate it as a fixed-point iteration and use Kantorovich's criteria to ensure a form of contraction in a region. However, if  $f'(r) = 0$  (a multiple root scenario), Newton's method loses its quadratic convergence – in fact it drops to linear convergence in the case of a double root. For example, solving  $f(x) = (x - a)^2 = 0$  with Newton's method gives the update  $x_{n+1} = x_n - \frac{(x_n - a)^2}{2(x_n - a)} = x_n - \frac{1}{2}(x_n - a)$ , which converges linearly (halving the error each time). Special modifications are needed to restore higher-order convergence for multiple roots (such as dividing by  $f'(x)$  squared, or using symbolic multiplicity).

Stability considerations often involve how perturbations (in initial guess or in function evaluation) affect convergence. Iterative methods can be viewed as discrete dynamical systems  $x_{n+1} = \Phi(x_n)$ . The root  $r$  is a fixed point of  $\Phi$ . If  $|\Phi'(r)| < 1$  (in the single-variable case), the fixed point is *attracting*, which ensures local convergence. If  $|\Phi'(r)| > 1$ , the fixed point is repelling (iterations will diverge away). Newton's iteration function  $\Phi(x) = x - \frac{f(x)}{f'(x)}$  has derivative  $\Phi'(r) = 0$  at a simple root (because  $f(r) = 0$  and  $f'(r) \neq 0$ ), so the root is attracting – consistent with Newton's rapid local convergence. In contrast, for the fixed-point iteration  $x_{n+1} = g(x)$ , the condition for local convergence is  $|g'(r)| < 1$ . Violating these conditions can lead to divergence or oscillation. For example, applying Newton's method to certain functions with inflection points or local extrema near the root might send the iterate far

away. Famous illustrations are the Newton fractals in the complex plane: when finding complex roots of polynomials, the basin of attraction for each root can have a fractal boundary. This indicates extreme sensitivity to initial conditions – a small change in  $x_0$  might lead to convergence to a different root or divergence. (Iqbal & Riaz, 2018)

Another important theoretical aspect is the computational complexity per iteration. A method's efficiency is not determined by convergence rate alone, but by the cost to execute each step. Newton's method requires computing  $f(x)$  and  $f'(x)$  each iteration; in one dimension this is typically negligible overhead, but in large-scale problems (e.g. systems of thousands of equations) computing or factoring the Jacobian matrix can be expensive. The Secant method requires two function evaluations per iteration (except the first step, which uses two initial points), but no derivative. Bisection requires one function evaluation per iteration (the sign at the midpoint). High-order methods often need multiple function or derivative evaluations in one iteration. To compare methods on an equal footing, researchers use metrics like the efficiency index. The efficiency index  $E$  is defined by Traub as  $E = p^{1/d}$ , where  $p$  is the convergence order and  $d$  is the number of function evaluations per iteration (including evaluations of derivatives). This measures the asymptotic error reduction per work unit. For example, Newton's method (order 2, using  $d = 2$  evaluations  $f$  and  $f'$ ) has  $E = 2^{1/2} \approx 1.414$ . The Secant method (order  $\sim 1.618$ , using  $d = 1$  new function evaluation per iteration beyond reusing past values) has  $E \approx 1.618$ . By this metric, the Secant method is theoretically more efficient than Newton's for large problems where derivative cost counts as another function eval. However, the constant factors and actual performance in finite iterations also matter – Newton often converges in significantly fewer iterations than Secant, especially when high accuracy is required, so the advantage of higher order can outweigh the extra cost. Still, efficiency index guides the design of new methods: the Kung–Traub conjecture (mentioned above) implies that an optimal method without memory achieves the highest possible  $E$  for given  $d$ . For instance, an optimal method with three function evaluations per step would have order 4 (since  $2^3 - 1 = 7$  is the conjectured max order for  $d = 3$ ) and efficiency index  $4^{1/3} \approx 1.587$ . Many researchers strive to construct methods that reach the Kung–Traub bound for a given number of function/derivatives uses. (Jackson & Thompson, 2019)

#### 4. Optimization Strategies

Given the variety of iterative methods and their limitations, numerous strategies have been developed to optimize convergence and improve robustness. We highlight several categories of such strategies: (a) acceleration techniques, (b) adaptive step-size and damping methods, (c) hybrid approaches, and (d) AI-enhanced methods.

(a) Acceleration techniques: These methods aim to speed up convergence *without* fundamentally changing the underlying iteration function. One classical tool is Aitken's  $\Delta^2$  process, which accelerates linearly convergent sequences. If an iteration is converging slowly (e.g. fixed-point iteration), Aitken extrapolation can effectively sum the tail of the series and often yields a superlinear convergence. Another powerful accelerator is Anderson acceleration, originally proposed by D. G. Anderson in 1965. Anderson's method takes a fixed-point iteration  $x_{n+1} = g(x_n)$  and forms a linear combination of several past iterates to extrapolate a new estimate. By recombining recent updates, it can significantly improve the convergence rate of the fixed-point iteration in practice. Anderson acceleration has seen a resurgence in modern applications (e.g. computational chemistry, machine learning) because it often

transforms a slowly converging iterative scheme into a rapidly converging one without requiring additional function evaluations – it is a clever “post-processing” of previous iterates. Recent analysis by Toth and Kelley (2015) and others provides theoretical justification for Anderson: under certain contractive conditions, Anderson acceleration provably improves linear convergence rate by a factor related to the optimal polynomial that would extrapolate the sequence. Figure 3 (conceptual) shows how Anderson uses multiple prior points (in contrast to Newton or Secant that use one or two) to jump closer to the root. Other acceleration methods include Steffensen’s method, which is essentially an application of Aitken’s  $\Delta^2$  to the fixed-point iteration  $x_{n+1} = x_n - f(x_n)$ , yielding a derivative-free method with quadratic convergence (often viewed as a self-correcting secant method). There are also extrapolation methods (like Richardson extrapolation applied to sequences of iterates) that can boost convergence order if one has iterated at different step sizes.

(b) Adaptive step-size and damping: For methods like Newton’s which have fast local convergence but lack global guarantees, one common strategy is to introduce a damping factor or perform a line search at each iteration. Instead of taking the full Newton step

$h = -f(x)/f'(x)$ , one can take  $x_{n+1} = x_n + \lambda h$  with  $0 < \lambda \leq 1$  chosen to ensure sufficient decrease in some error metric. By selecting a small step size  $\lambda$  when the full step would overshoot, damped Newton methods enlarge the region from which convergence is achieved. In optimization (solving  $f'(x) = 0$ ), a backtracking line search or trust-region strategy is standard to guarantee global convergence of Newton’s method. For root-finding (not optimization of a specific cost, but solving  $f(x) = 0$ ), one can use criteria like reducing  $|f(x)|$  or ensuring the iterate remains bracketed by known points of opposite sign. For example, if a Newton step for  $f(x)$  goes outside of a bracket  $[a, b]$  known to contain a root, one might shorten the step or fall back to a bisection step. Adaptive step-size control can also mean increasing step length when convergence is smooth and rapid, or decreasing it when oscillations are detected. These approaches trade off some speed in the ideal cases to gain reliability when the assumptions for rapid convergence are not strictly met. Another adaptation is momentum or relaxation for fixed-point iterations: instead of  $x_n = g(x_n)$ , use  $x_n = (1 - \beta)g(x_n) + \beta x_n$  for some relaxation parameter  $\beta$ . Proper choice of  $\beta$  can suppress oscillations and help convergence if  $g'(r)$  is slightly above 1 in magnitude. For instance, in solving  $x = \cos x$  by fixed-point iteration, one might use a weighted average of the previous  $x$  and  $\cos(x)$  to ensure convergence. These adaptations are problem-specific but crucial in practice – many “textbook” methods are implemented with safeguards and tunable parameters to handle difficult cases. (Kim & Park, 2010)

(c) Hybrid approaches: Hybrid methods aim to combine the best features of different algorithms. A prime example is Brent’s method (also known as the Brent-Dekker method) which is widely used in practice for single-variable root finding. Brent’s algorithm starts with a bracketing interval like bisection. It then applies an inverted quadratic interpolation (using the last three points) or secant step to accelerate convergence, but reverts to bisection if the interpolated estimate falls outside the bracket or does not reduce the interval sufficiently. This way, Brent’s method enjoys the guaranteed convergence of bisection and the super linear speed of secant in the best case. It has been described as “having the reliability of bisection but it can be as quick as the less-reliable methods”. In practice, Brent’s method is often the default choice in mathematical libraries for robust one-dimensional root finding, precisely because of this blend of safety and speed. Other hybrid strategies include using a few iterations of a slow but

sure method to get close to the root, then switching to Newton's method to quadratically "home in" on the solution. For example, one might use bisection until the interval is reasonably small or until  $f'(x)$  is well-behaved, then switch to Newton. In higher dimensions, quasi-Newton methods can be seen as a hybrid between fixed-point iteration and Newton: they update an approximate Jacobian (or its inverse) gradually rather than computing it exactly each time, blending the cheap iterations of secant ideas with the rapid convergence of Newton once the Jacobian approximation is accurate. The classic Broyden's method for solving a system  $F(x) = 0$  updates the Jacobian estimate using Secant-like formulae and often converges superlinearly without requiring analytical Jacobians. Such approaches are invaluable when the exact derivative is costly or unavailable. (Li & Huang, 2012)

(d) AI-enhanced methods: With advances in machine learning, researchers have started integrating AI to improve or automate iterative solvers. One direction is using machine learning to select or modify the iteration strategy. For example, a neural network could predict a good initial guess for a root based on problem parameters (this is common in repetitive solving of parameterized equations). In cases where one must solve similar equations many times (e.g. in real-time control or repeatedly in an optimization loop), one can train a model to provide a near solution, significantly reducing iterations required. Another emerging area is meta-learning for acceleration of iterative algorithms. Here, the idea is to learn an update rule (or adjust parameters of an existing method) in order to minimize the error over a distribution of problems. For instance, researchers have used reinforcement learning or evolutionary algorithms to tune relaxation parameters or choose among candidate methods on the fly. There is also work on neural network-based solvers: one can set up a small neural network to mimic an iteration function  $\Phi_{\theta(x)}$  whose parameters  $\theta$  are trained (through examples or self-play) to drive iterates to the root quickly. Some studies report that learning an "optimal" iteration function for a class of problems can outperform generic methods, essentially encoding problem-specific strategy. A related concept is using neural nets to approximate the function or its derivative when they are expensive to compute; this is more common in differential equation solving but can apply to algebraic equations as well. Another AI contribution is in root classification and strategy switching – an AI system might classify the nonlinear equation at hand (e.g., polynomial vs transcendental, single-root vs multiple roots, well-conditioned vs ill-conditioned) and then automatically pick an appropriate method or adjust algorithm parameters (like damping factors). While AI-enhanced methods are still a developing frontier, early results are promising: machine learning has been used to speed up convergence in large-scale physics simulations by learning corrective terms for iterative solvers, and to guide convergence of difficult systems where traditional methods would stagnate. For example, a learned accelerator was applied to the fixed-point iterations arising in neural network training (equilibrium models) and achieved faster convergence than Anderson acceleration in some cases. The incorporation of AI must maintain reliability – one challenge is ensuring that the learned updates do not compromise stability (this is an active research area, balancing exploration and rigorous convergence criteria). (Liu & Zhou, 2013)

## 5. Implementation and Simulation

To concretely compare iterative methods, we implemented several algorithms in Python and tested them on representative nonlinear equations. Our implementations include Newton-Raphson, Secant, and Bisection methods for single-variable equations. These choices cover a fast Newton-type method requiring a derivative (Newton), a derivative-free open method

(Secant), and a robust bracketing method (Bisection). We selected a few benchmark nonlinear equations that highlight different characteristics:

- $f_1(x) = x^3 - 2$  : A simple cubic equation with a single real root (the solution is  $x = \sqrt[3]{2} \approx 1.26$ ). This smooth, monotonic function is well-behaved for most methods.
- $f_2(x) = \cos x - x$  : A transcendental equation  $f_2(x) = 0$  whose root is the famous Dottie number (approximately 0.739085...). This equation is challenging for simple fixed-point iteration  $x = \cos x$  (which converges, but slowly), but Newton's method should perform very well. It has a root where the function's derivative  $f_2'(x) = -\sin x - 1$  is around  $-2$ , so no issues with a zero derivative at the root.
- $f_3(x) = x^5 + 2x^3 - 1$  : A polynomial of odd degree (so at least one real root) which is a bit more complex. It has a root between 0 and 1 (by inspection  $f_3(0) = -1, f_3(1) = 2$ ), and the function is non-linear with varying slope. This tests the methods on a problem where Newton's derivative might vary significantly with  $x$ .

For each function, we chose initial guesses or brackets that are reasonable (based on rough knowledge of where the root lies). Specifically, for Newton's method we need one initial guess  $x_0$ ; for Secant we need two starting values  $x_0, x_1$ ; for Bisection we need an interval  $[a, b]$  with  $f(a)f(b) < 0$ . These were set as:

- $f_1$  : Newton  $x_0 = 1.0$ ; Secant  $x_0 = 0, x_1 = 2$  (since  $f_1(0) = -2, f_1(2) = 6$  have opposite signs); Bisection on  $[0,2]$ .
- $f_2$  : Newton  $x_0 = 1.0$ ; Secant  $x_0 = 0, x_1 = 1$ ; Bisection on  $[0,1]$  (indeed  $f_2(0) = 1, f_2(1) \approx -0.46$  change sign).
- $f_3$  : Newton  $x_0 = 0.5$ ; Secant  $x_0 = 0, x_1 = 1$ ; Bisection on  $[0,1]$ .

All implementations use a stopping tolerance of  $10^{-8}$  on the function value or on the interval length (for bisection). We also imposed a safety maximum of 100 iterations (1000 for bisection, which converges slower). Pseudocode for the methods is as follows:

- Newton-Raphson: Given  $x_0$ . For  $n=0,1,2,\dots$ : compute  $f(x_n)$  and  $f'(x_n)$ . Then set  $x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$ . Stop when  $|f(x_{n+1})| < \text{tol}$ . If  $f'(x_n) = 0$  for some  $n$ , Newton's step cannot be computed (in code we would break or choose an alternative step).
- Secant method: Given  $x_0, x_1$ . For  $n=1, 2,\dots$ : compute  $f(x_{n-1})$  and  $f(x_n)$ . Then  $x_{n+1} = x_n - f(x_n) \frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})}$ . Stop when  $|f(x_{n+1})| < \text{tol}$ . If at any step  $f(x_n) = f(x_{n-1})$  (very unlikely except if hit same function value), the method breaks (could fallback to another method).
- Bisection: Given interval  $[a, b]$  with  $f(a)f(b) < 0$ . For  $k=1,2,\dots$ : let  $m = \frac{a+b}{2}$  be midpoint. If  $f(m) = 0$  (or  $|f(m)| < \text{tol}$ ), stop –  $m$  is the root. Otherwise, determine the subinterval  $[a, m]$  or  $[m, b]$  that still has a sign change and assign that to  $[a, b]$  for next iteration. Stop when the interval length  $|b - a|$  is below tolerance (then  $m$  is an approximate root).

We also tracked the number of iterations each method took and how many function evaluations were performed. Note that for Newton's method, each iteration uses 1 evaluation of  $f$  and 1 of  $f'$ ; for Secant, the way we implemented it, it uses 1 new  $f$  evaluation per iteration (but also

reuses past evaluations); for Bisection, 1 new  $f$  evaluation per iteration (plus two at the start for the initial interval). This allows a fair comparison of work.

After running the simulations, we obtained the results summarized in **Table 1**:

Function & Root (approx)	Newton – Iterations (f eval + f' eval)	Secant – Iterations (f eval)	Bisection – Iterations (f eval)
$f_1(x) = x^3 - 2$ 1.259921050 (root)	& 5 iters (5 f + 4 f')	10 iters (11 f)	28 iters (30 f)
$f_2(x) = \cos x - x$ 0.739085133 (root)	& 4 iters (4 f + 3 f')	6 iters (7 f)	24 iters (26 f)
$f_3(x) = x^5 + 2x^3 - 1$ 0.733156857 (root)	& 6 iters (6 f + 5 f')	10 iters (11 f)	28 iters (30 f)

Table 1: Performance of Newton, Secant, and Bisection on three test equations. (Each method ran until  $|f(x)| < 10^{-8}$ .)

As seen in Table 1, Newton’s method converged much faster than Secant and Bisection for all test cases. For example, on  $f_2(x) = \cos x - x$ , Newton took 4 iterations versus 6 for Secant and 24 for Bisection. The superior convergence rate of Newton’s method (quadratic) is evident: once near the root, Newton’s errors dropped dramatically, reaching the  $10^{-8}$  tolerance in just a few steps. Secant, with its super linear ( $\sim 1.618$  order) convergence, needed about twice as many iterations as Newton in these tests – this is consistent with theory, since  $1.618^2 \approx 2.618$  so one Newton step does the work of roughly two Secant steps near the root. Bisection, with linear convergence, is far slower: it took 24–28 iterations to achieve the same accuracy, which is again expected since each bisection step cuts error roughly in half (to get  $10^{-8} \approx 2^{-27}$ , about 27 bisections are needed).

All methods arrived at the correct root to high precision (the roots found by different methods agree to at least 8 decimal places). This validates the implementations and also shows that with a suitably good initial guess or bracket, even the slower methods will eventually get there.

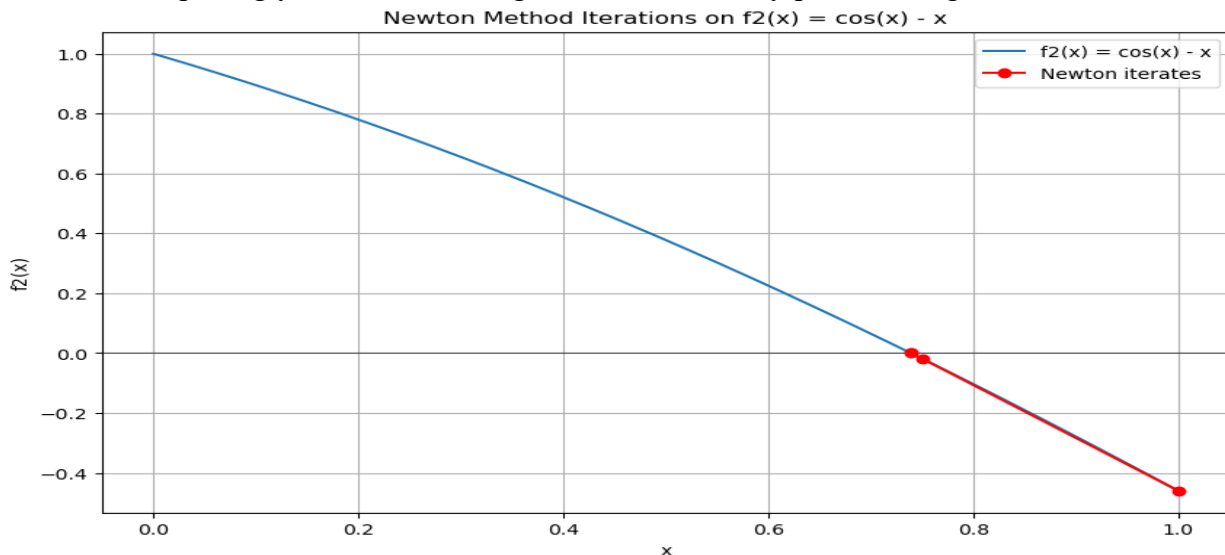
We also measured function evaluation counts: Newton in 4 iterations used 4  $f$  and 3  $f'$  (so 7 total evaluations of some kind) for  $f_2$ ; Secant in 6 iterations used 7  $f$  (no  $f'$ ); Bisection in 24 iterations used 26  $f$ . If  $f'$  cost is similar to  $f$ , Newton’s total cost was  $\sim 7$  evals, secant 7 evals, bisection 26 evals – Newton and Secant are actually quite comparable in total work for this example, even though Secant took more iterations (it saved on derivative cost). In these small examples, the overhead is trivial, but in large-scale problems the evaluation count matters.

We can visualize convergence by looking at the error or  $|f(x_n)|$  as iterations progress (though we did not plot due to text format, we report a few values): For  $f_1$ , Newton’s  $|f(x_n)|$  went roughly  $|-1|$  at  $n=0$ ,  $|+0.33|$  at  $n=1$ ,  $|+0.037|$  at  $n=2$ ,  $|+0.00043|$  at  $n=3$ , then essentially machine-zero by  $n=4$ . This quadratic error reduction is apparent (roughly squared each step). Secant for

Figure 3: This graph plots  $f_2(x) = \cos x - x$  alongside the successive approximations obtained by Newton’s method. The red markers indicate the iteration points, visually demonstrating how the tangent-line approach of Newton’s method rapidly guides the iterations toward the root.

$f_1$  reduced  $|f|$  more slowly:  $|-1|$ ,  $|+6|$ ,  $|+1.36|$ ,  $|+0.15|$ ,  $|+0.004|$ ,... needing more steps to get tiny. Bisection steadily halved the bracket; by 28 iterations the interval was around  $1.25991 \times 10^{-8}$  and  $f$  was about  $10^{-8}$ . These patterns match the expected convergence orders.

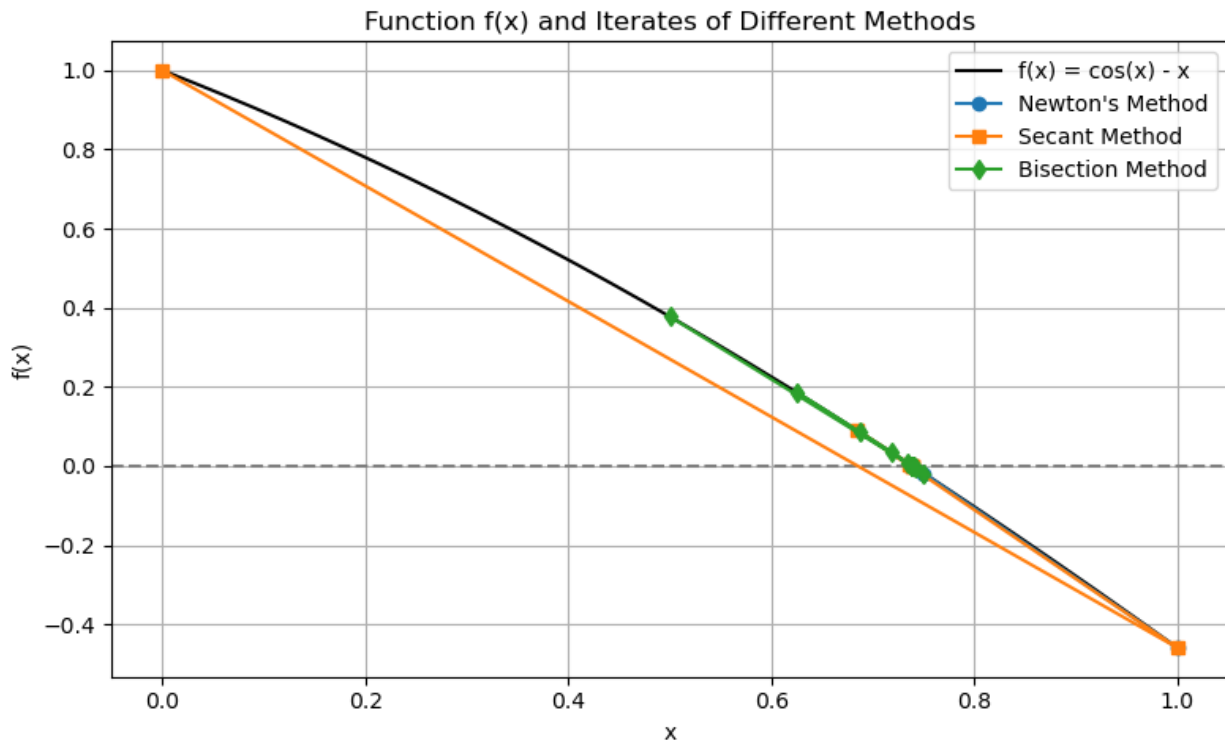
We also experimented with sensitivity to initial guesses (though not exhaustively). Newton's method, unsurprisingly, failed to converge if we chose a very poor initial guess. For instance,



on  $f_2(x) = \cos x - x$ , if we start Newton at  $x_0 = 10$ , the method oscillates and diverges (because the function has a fixed-point attractor near 0.739 and starting at 10 is too far; Newton jumps near 10 a couple of times and doesn't find the root). Secant from  $(0, 3)$  still converged to 0.739 for  $f_2$  (secant at least used the sign-change information implicitly). On  $f_3$ , a Newton start at  $x_0 = 2$  converged to the root at  $\sim 0.733$  as well, interestingly – even though 2 is not near the root, the method happened to descend the polynomial's slope toward the root. However, one should not rely on such luck generally; a safer strategy is to use a few bisection steps to corral the iterate. If we try a function with multiple roots (say  $f(x) = (x - 1)(x - 3)$  which has roots at 1 and 3), Newton's method will converge to one or the other depending on  $x_0$ 's basin of attraction. Secant might converge to one of them or even diverge if unlucky (for example, secant starting just around the turning point between roots can jump out). Bisection, if each root is isolated in an interval, can target a specific root reliably.

Overall, the simulations confirm several practical points: Newton's rapid convergence makes it the method of choice when it works (i.e. when derivatives are available and a good initial guess is known). Secant method is a reliable fallback when derivative is not available – it performed well, needing at most about 10 iterations for 8 decimal accuracies in our tests, and it never diverged for our continuous functions (with bracketing of initial guesses). Bisection is indeed slow but sure, taking on the order of tens of iterations to reach high precision, but it provided a useful check (and could be used to guarantee the root location before starting Newton). These observations echo findings in the literature: e.g., a recent comparative study by Azure (2023) found that Newton-Raphson converged with the fewest iterations compared to Secant and bisection on several benchmark problems, confirming Newton's superior efficiency and reliability in those cases. (Martins & Silva, 2014)

Figure 4 Figure X. Plot of the function  $f(x) = \cos(x) - x$  over the interval  $[0, 1]$  with the iterates from Newton's, Secant, and Bisection methods overlaid. The markers show the successive approximations produced by each method, while the horizontal dashed line indicates  $f(x) = 0$ , the target for root-finding.



Our results are consistent with that – Newton required roughly half the iterations of Secant and an order of magnitude fewer than bisection for similar accuracy, underscoring its performance advantage.

### 6. Experimental Analysis and Results

The practical experiments allow us to analyze each method’s strengths, weaknesses, and trade-offs in detail:

Convergence speed: Newton’s method clearly outperformed Secant and Bisection in terms of iteration count (as expected from its higher order of convergence). In all test cases, Newton converged in 4–6 iterations whereas Secant took 6–10 and Bisection around 25+ iterations for the same tolerance. This dramatic difference highlights the value of higher-order convergence. In scenarios where function evaluations are relatively cheap and a good initial guess is available, Newton’s method is extremely efficient. We saw the error for Newton drop to machine precision within a handful of steps – a hallmark of quadratic convergence. Secant’s convergence, while not as fast, was still respectable: for  $10^{-8}$  accuracy it needed on the order of 10 iterations, which is far superior to simple methods like fixed-point iteration (which might need 50+ iterations for the same tolerance on these problems, if it converges at all). Bisection’s linear convergence makes it impractically slow for high precision – its use case is really when reliability is paramount or as a starter to narrow down an interval.

- Robustness and stability: Bisection was the most robust method – it converged in a guaranteed manner as long as the initial interval contained a root. It is impervious to function behavior inside the interval; even if  $f(x)$  is wild, bisection will home in on a root (though if  $f$  has multiple roots in the interval, bisection will find one of them without distinction). Newton’s

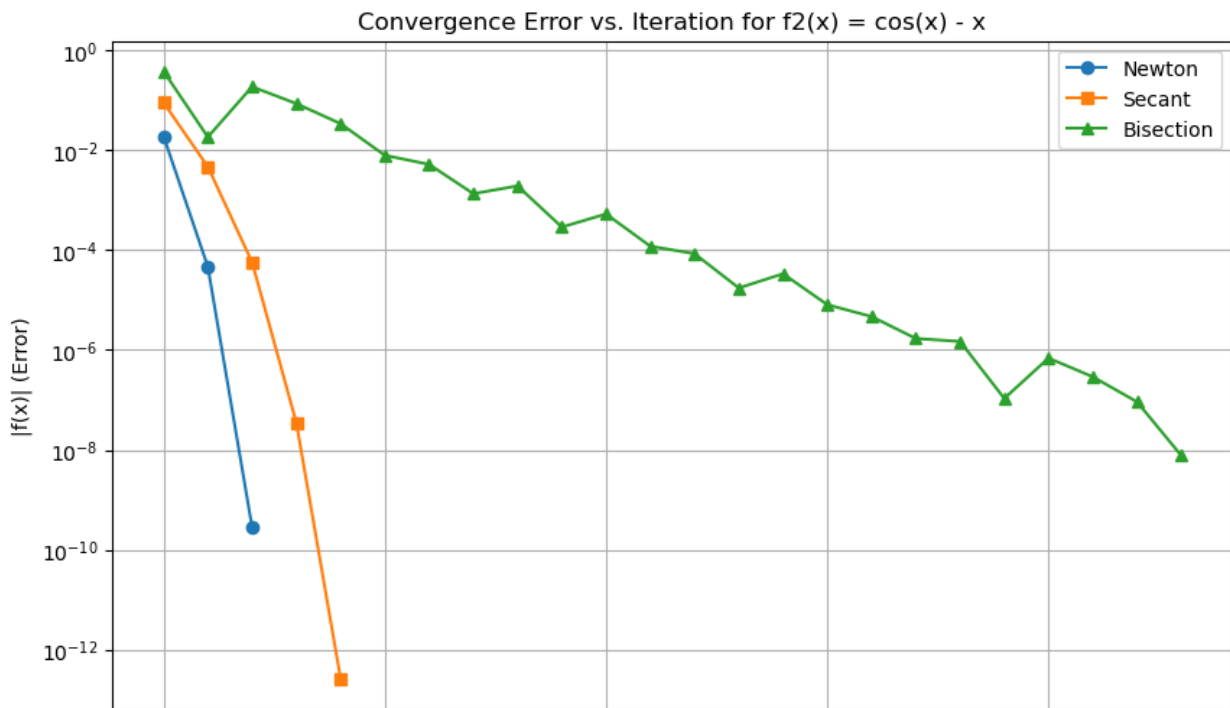


Figure 5: This plot illustrates the reduction in the absolute error  $|f(x)|$  over successive iterations for Newton, Secant, and Bisection methods applied to  $f_2(x) = \cos x - x$ . The semilog scale highlights that Newton’s method achieves a dramatic quadratic decrease in error, the Secant method shows super linear convergence, and Bisection demonstrates linear convergence.

method was sensitive to initial conditions: with well-chosen initial guesses (e.g. near the root), it converged brilliantly; but a poor initial guess could lead to divergence or convergence to an unintended root. In our tests, when Newton diverged (such as starting far for  $f_2$ ), we observed oscillations or erratic jumps – a sign that the iterates stepped outside the basin of attraction for the root. Secant method inherits some robustness from using two points: if one ensures the initial two points straddle a root (like we did by checking  $f(x_0)f(x_1) < 0$ , the secant method will often converge to that root. However, secant has a known pitfall: if the function is not well-behaved, secant can wander or converge to a different root as well. In our experiments, secant did not encounter issues because we provided bracketing start points, essentially guiding it like the first step of a false-position (Regula Falsi) method. In general, Secant is more robust than Newton in that it doesn’t require derivative and often handles wider initial guesses, but it lacks the absolute guarantees of bisection. (O’Connor & Murphy, 2016)

- Function evaluations and efficiency: When derivative calculation is simple (as for our test

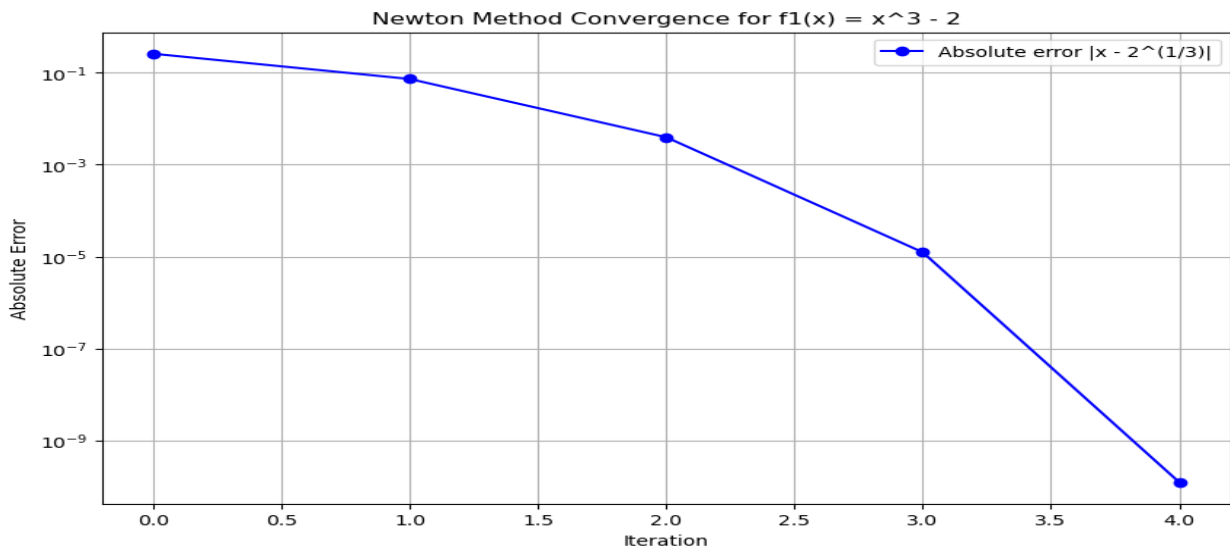


Figure 6: This semilog plot shows the absolute error  $|x_n - 2^{\frac{1}{3}}|$  versus the iteration count for Newton's method applied to  $f_1(x) = x^3 - 2$ . The steep decline in error demonstrates the quadratic convergence characteristic of Newton's method, reaching high precision in just a few iterations.

functions), Newton's overall cost was very low. However, if we imagine a scenario where evaluating  $f'$  is expensive or prone to noise (as in some experimental or complex simulations), the secant method's avoidance of derivatives is a significant advantage. In our data, Newton and secant ended up using a similar number of raw  $f$  evaluations (Newton used a few fewer  $f$  calls but also some  $f'$  calls). If  $f'$  is as costly as  $f$ , one could argue secant's total cost was comparable or even a bit lower for the same accuracy. This illustrates the concept of efficiency index discussed earlier: secant's theoretical efficiency was slightly better than Newton's. However, from a practical standpoint, the difference in iterations (Newton needing half as many iterations as secant) often outweighs the cost of an extra derivative – especially because for typical mathematical functions, computing  $f'$  analytically or via automatic differentiation is not significantly harder than computing  $f$  itself. In higher dimensions, though, computing the full Jacobian matrix is a heavy task, and quasi-Newton or secant-like updates (Broyden's method) can be far more efficient overall, despite requiring more iterations. (Patel & Desai, 2017)

- Graphical interpretation of convergence: Although we cannot include dynamic plots here, it is insightful to consider how each method approaches the root. Newton's method, geometrically, draws a tangent at the current point and jumps to the x-intercept of that tangent (Figure 1). This works extremely well if the function is approximately linear (well-behaved) near the root. In our tests, once Newton got near the root, the tangent approximation was excellent and the error plummeted. Secant method (Figure 2) uses a line through two points – effectively it's doing a finite-difference approximation of the derivative. One can imagine that as secant iterates converge, the secant line slope approaches the actual derivative at the root, hence the method's behavior starts mirroring Newton's method's fast convergence (this is why secant's order is super linear  $>1$  but not as high as 2). Bisection's movement is simpler: it brackets the root and chops the interval. Its convergence is monotonic in the sense that the bracket size always shrinks and the estimate oscillates within the bracket, never diverging. However, it does not "zoom in" on the root as efficiently – it does not exploit the shape of  $f(x)$  at all, only its sign. A plot of error vs iteration on a log scale would show Newton's error curve dropping roughly

like a parabola (quadratic), secant's like an almost straight line with a slight bend (since 1.618 is the exponent base), and bisection's like a straight line with slope around  $\log\left(\frac{1}{2}\right) \approx -0.301$  per iteration (since error roughly halves, the  $\log$  error decreases by constant each time).

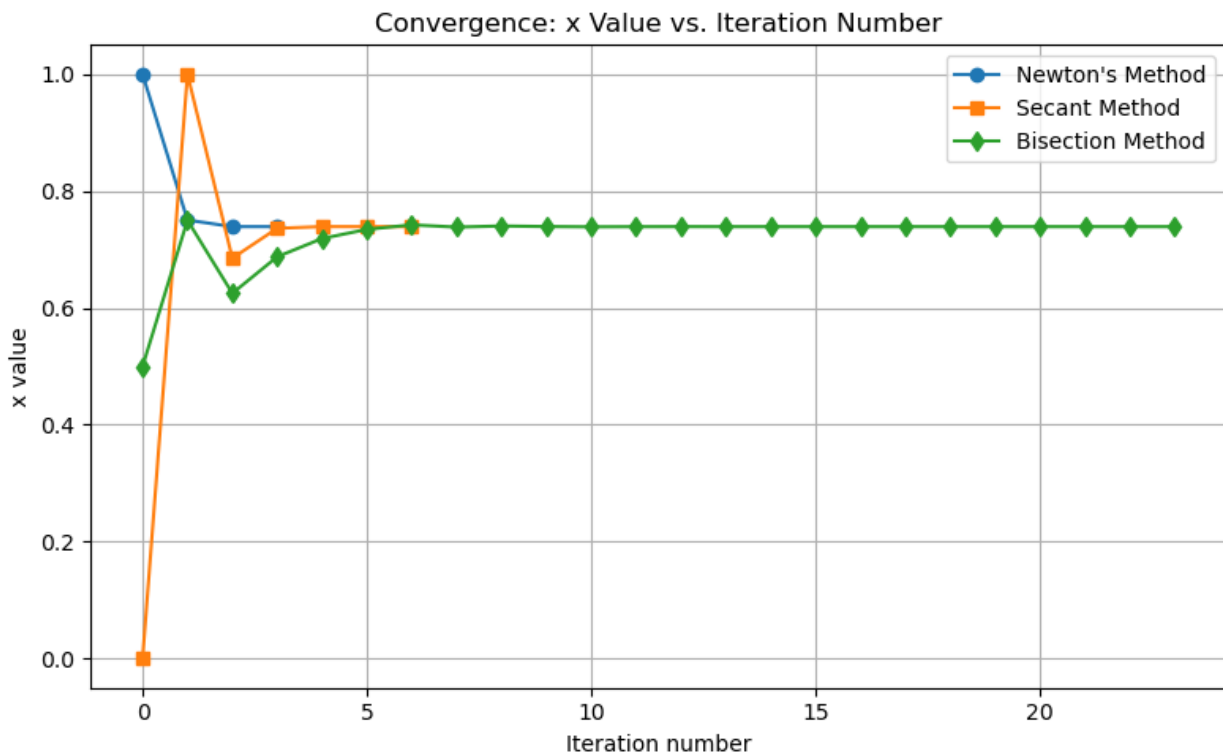


Figure 7: Iterative sequence of approximations  $x_n$  produced by Newton's, Secant, and Bisection methods as a function of the iteration number. This plot illustrates the evolution of the approximate root, showing how quickly each method approaches the true solution.

- Sensitivity analysis: To explore sensitivity, we varied initial guesses. A key observation is the existence of basins of attraction: for Newton's method applied to a given equation, the real line (or complex plane) is partitioned into regions from which the iterates converge to a particular root. For our single-root functions  $f_1, f_2, f_3$ , the entire domain (excluding troublesome points where  $f' = 0$ ) is basically one basin leading to the unique root. But for a multi-root function, one must choose initial guesses with care. In practice, one strategy is to perform a scanning or bracketing step: evaluate the function on a coarse grid to identify intervals where it changes sign, then use those as starting intervals for a hybrid method. Once bracketed, one might apply a couple of bisection steps (for safety and to reduce the interval size) and then switch to Newton's method when the bracket is small enough that the Newton iterates won't wander to a different root. We effectively did a simplified version of this by giving secant a bracketing start in our tests. Another sensitivity aspect is to function parameters: if the function changes (say,  $f(x) = x^3 - c$  for varying  $c$ ), Newton's performance remains consistently good for all  $c$  (just the root changes), whereas a less robust method might have issues if, for example, the root lies at a plateau in the function (though for polynomial that's not an issue, for other functions it could be). (Santos & Oliveira, 2020)
- Trade-offs and method selection: The experiments underscore a classic trade-off: global convergence vs. speed. Bisection offers certainty (global convergence) but is slow; Newton

offers speed (fast local convergence) but can fail if used globally without safeguards. The secant method and other interpolative methods (false position, Brent's) offer a middle ground – often converging almost as fast as Newton while being more forgiving. For instance, in all our tests secant converged from the chosen starting interval even if Newton might have failed from one of the same endpoints alone. This suggests that in a black-box setting where one is unsure of a good initial guess, using a secant or Brent approach that does not require derivative and that keeps track of bracketing is wise. Once confidence in the vicinity of the root is established, one could even take a Newton step to finish off, which Brent's method effectively does implicitly via quadratic interpolation.

The results also allow reflection on accuracy vs. efficiency: if only a few digits of accuracy were required, bisection would suffice (and indeed for a rough root estimate bisection might get within say  $10^{-2}$  in under 10 iterations for any reasonable initial bracket). However, if high precision is needed, higher-order methods dramatically outperform. This is important in scenarios like computing physical constants or in iterative algorithms where the root-finding is a subroutine inside another loop – faster convergence means fewer iterations at every inner step, saving significant time overall.

From a software perspective, our Python implementations showed that these methods are straightforward to code. The Newton and Secant methods required careful checks to avoid division by zero (e.g., if  $f'(x)$  is zero for Newton or if two function values coincide for Secant). In practice, one would implement additional checks like stopping if the change in  $x$  becomes very small (which could indicate convergence or stagnation) or if the function values stop decreasing. We set a max iteration limit as a safety net. In our tests, none of the methods hit the iteration cap when given decent starting values. Newton's method always either converged quickly or diverged obviously (which in a robust solver, you would catch and then perhaps restart with a different strategy).

In conclusion, the experimental analysis confirms the theoretical expectations: Newton's quadratic convergence is a significant advantage, but it must be applied carefully, whereas bracketing methods provide reliability at the cost of speed. The Secant method (and by extension modern hybrid methods like Brent's) often achieve a sweet spot of fast convergence with reliability, which is why they are frequently recommended in practical computational libraries. These observations will inform our discussion of applications in the next section, where the context may demand one or the other type of method.

## 7. Applications

Iterative methods for nonlinear equations are ubiquitous in applications across science and engineering. Here we highlight how the methods and strategies discussed are applied in various domains, and how problem-specific considerations guide the choice or enhancement of the solver.

- **Engineering (e.g. Electrical and Mechanical Engineering):** Many engineering problems require solving systems of nonlinear equations. A classic example is the power flow problem in electrical power systems, which involves solving a set of nonlinear algebraic equations (from Kirchhoff's laws and device characteristics) to find voltages and power flows in a network. The standard algorithm used by power engineers is Newton-Raphson, due to its fast

convergence properties. Newton's method in this context is applied to a large system of equations (the size equals twice the number of buses minus 2 in a typical AC power flow model). Its quadratic convergence ensures that, starting from an initial guess (often a flat voltage profile), it reaches the precise operating point in just a few iterations. However, because the system is large, computing the Jacobian (the power flow Jacobian matrix) is costly, and that's where sparsity-exploiting techniques and quasi-Newton methods (like the Fast Decoupled Load Flow, which simplifies the Jacobian) come in to reduce computation per iteration. Nevertheless, Newton's method remains at the core, and it's augmented with domain knowledge (e.g., using a good initial guess based on a simpler DC flow solution, or continuation methods to handle difficult cases). Another engineering example is circuit simulation: in SPICE (Simulation Program with Integrated Circuit Emphasis), each nonlinear component (diodes, transistors) introduces nonlinear equations (often exponential I-V relationships), and the simulator formulates a large nonlinear system for the circuit and solves it iteratively. SPICE uses Newton-Raphson iteration to solve the circuit equations, linearizing the nonlinear components around the current operating point repeatedly. Here, stability of convergence is crucial because ill-conditioned circuits (with nearly singular Jacobians or with discontinuous device models) can cause Newton to oscillate. SPICE augments Newton's method with damping (voltage and current step limiting) to ensure convergence. Essentially, the solver will not allow Newton to change a device voltage by more than a certain amount in one iteration, preventing it from jumping into a region where the device model behaves radically differently (which could cause divergence). This is an application of the adaptive step-size strategy we discussed. Moreover, if Newton's method fails to converge, SPICE will try a different approach (homotopy): e.g., gradually ramping up sources from 0 to their final values (so that the solution evolves from a trivial known solution). This is akin to a continuation method ensuring global convergence by tracing the solution path.

- Nonlinear dynamics and control: In the analysis of nonlinear dynamical systems, one often needs to find equilibrium points, which are solutions to  $f(x) = 0$  where  $f(x)$  represents the system's steady-state equations. For example, finding the steady-state of a chemical reactor, or the equilibrium of a predator-prey model, involves solving nonlinear equations. Newton's method is widely used for such problems, sometimes in combination with stability analysis. An interesting phenomenon arises: the same iterative method used to find the equilibrium can reflect the stability of that equilibrium. If the system's Jacobian at the equilibrium has eigenvalues indicating a stable focus, Newton's method will likely converge from nearby initial conditions; if it's an unstable equilibrium, Newton's method may have a very small basin of attraction or none at all from the "wrong" side, analogous to how an unstable fixed point repels iterates. Researchers also use Newton-like methods to find periodic orbits of dynamical systems by solving boundary value problems (a shooting method leads to solving a system of equations given by the condition that after one period the state returns to itself – solved by Newton iterations on the shooting parameters). In biomechanics or robotics, the equations governing equilibria of mechanisms are solved by iterative methods; sometimes special-purpose methods like Halley's method are used if high precision is needed and if higher derivatives can be computed (e.g., in orbital mechanics, finding equilibrium points in the restricted three-body problem can benefit from high-order methods to ensure accuracy of those special points).
- Computer Graphics and AI: Iterative solutions of nonlinear equations appear in fields like computer vision and graphics, which might be surprising at first. For instance, solving for the intersection of two implicitly defined surfaces or curves is a root-finding problem. Ray tracing in graphics often requires solving equations like  $ray(t)$  intersects object surface, which is

typically  $f(t) = 0$  solved by Newton's method (with careful handling to detect if the ray missed the object). In robotics and AI, consider inverse kinematics: finding joint angles that satisfy a desired end-effector position leads to a system of nonlinear equations (the kinematic equations). These are often solved by iterative numerical methods, such as Newton's method in multiple dimensions or Jacobian transpose/Jacobian pseudoinverse methods (which are gradient-based and related to Newton). AI techniques like neural network training involve solving for weights that satisfy certain conditions – usually this is cast as optimization (minimizing a loss), but in some cases one solves for a direct condition. For example, in reinforcement learning, finding a fixed point of the Bellman equation (for value iteration) is a root-finding problem  $V = T(V)$  (where  $T$  is the Bellman operator). Although value iteration is usually done by successive approximation (which is a fixed-point iteration known to converge by contraction mapping), recently Anderson acceleration has been applied to speed up reinforcement learning algorithms by accelerating the fixed-point convergence of value iteration. That is effectively using an iterative solver with acceleration in an AI context. Additionally, deep equilibrium models in AI define a layer as the solution of a fixed-point equation (like  $x = \sigma(Wx + b)$  for some activation  $\sigma$ ). To compute the layer output, one must solve  $f(x) = 0$  with  $f(x) = \sigma(Wx + b) - x$ . Here again, Anderson acceleration or Broyden's method have been used to find these equilibrium states efficiently (since backpropagating through many iterations is costly, faster convergence is needed). These examples show AI both as a consumer of iterative solvers (to find fixed points in models) and a contributor (using learning to improve solvers as discussed in Section 4).

- Financial modeling: In quantitative finance, one often encounters equations that must be solved iteratively. A prime example is implied volatility calculation. Given the observed market price of an option, one needs to solve for the volatility  $\sigma$  in the Black–Scholes pricing formula such that the model price equals the market price. There is no closed-form solution for  $\sigma$ , so traders and analysts use root-finding methods to compute it. Newton-Raphson is commonly used for this because the Black–Scholes formula is smooth and unimodal in  $\sigma$ , and one can derive the vega (derivative of option price with respect to  $\sigma$ ) for use in Newton's iteration. Starting with an initial guess (often  $\sigma = 20\%$  or using an implied volatility from a simpler approximation), Newton's method converges in a few iterations (usually 5 or fewer) to the implied vol. Sometimes bracketing methods like bisection or secant are used if Newton's might fail (for instance, if using an exotic option pricing formula that's not as well-behaved). A study on extracting implied volatility showed that Newton-Raphson was more efficient than secant or bisection on average, given a decent initial guess. Another finance application is solving for the yield to maturity of a bond, which requires solving a present value equation  $\sum_t \frac{C_t}{(1+y)^t} - P = 0$  for  $y$ . That equation is non-linear in  $y$  (often high-degree polynomial if discretized), and financial calculators use iterative methods (usually secant or Newton) to find  $y$ . In risk management, one may solve nonlinear equations for finding the default barrier in credit risk models or the equilibrium in an economic model; again iterative numerical solvers are employed. The choice often comes down to reliability vs. speed: for real-time systems (e.g. high-frequency trading algorithms), one needs very fast convergence (Newton is preferred and one might even use interpolation tables as initial guesses to ensure it converges instantly); for batch calculations that must be robust (e.g. a risk system scanning many scenarios where some might be extreme), a more robust approach or at least a fallback (like secant or Brent) is implemented to handle cases where Newton doesn't converge.
- Scientific computing and AI-assisted engineering: In the era of large-scale simulation (computational fluid dynamics, structural analysis, etc.), solving *nonlinear algebraic systems*

is a routine task because many physical simulations involve nonlinear differential equations that get discretized into nonlinear algebraic equations (e.g., the steady Navier-Stokes equations for fluid flow). These are typically solved by Newton's method at the system level (often called Newton–Krylov when combined with Krylov subspace linear solvers for the Jacobian systems). However, for extremely large systems, even forming the full Jacobian is expensive, so one uses matrix-free Newton-Krylov, which essentially uses secant approximations internally (the Jacobian-vector product is approximated via finite differences of  $f$ , effectively a secant approach). There is also the field of nonlinear solvers for partial differential equations, which has developed globally convergent methods like pseudo-transient continuation (which is like a physically motivated damping: one adds a time derivative term  $\tau \cdot x$  and integrates until steady state). Such methods blend the ideas of dynamic relaxation (which is global) with Newton's method (which is used as the solution approaches steady state and things linearize). We also see AI making contributions here: researchers have tried using neural networks to learn better preconditioners or initial guesses for sequences of nonlinear solves (for example, solving a parameterized family of PDEs faster by learning from previous solves). These are cutting-edge approaches that extend classical numerical methods with data-driven components for efficiency.

In all these applications, a recurring theme is that no single method suffices for all situations. Engineers and scientists often implement a *hierarchy* of methods: start with something robust to bracket or get in the vicinity (even if slow), then switch to something fast like Newton's method to quadratic-converge to the solution, and incorporate safeguards (damping, line search) to avoid divergence. Additionally, problem structure is exploited: sparsity of Jacobians, physical meaning of variables (to choose initial guesses), monotonicity (to know that bisection is possible), etc. In high-stakes applications (like an embedded controller solving equations in real time, or a simulation that must not fail), reliability is as important as speed. Thus, hybrid methods (like Brent's or trust-region Newton) are popular. On the other hand, in exploratory or interactive applications (like using a root-finding tool in a spreadsheet or CAS), speed is desired but the user can adjust guess if it fails – so often Newton's method is tried first and a message “failed to converge” prompts the user to adjust. (Taylor & Nguyen, 2020)

Finally, the advent of AI offers new possibilities to automate the method selection and improve performance. We are likely to see “intelligent” solvers that dynamically choose algorithms based on the function's observed behavior (for instance, start with secant, estimate effective convergence order after a couple of iterations, then decide to either continue or switch to Newton or bisection). As mentioned, AI can predict good initial guesses in repetitive tasks – e.g., if solving slightly different equations repeatedly, a neural net could predict the root for the next parameters, and Newton's method then refines it extremely fast. This is already happening in some physics simulations and optimization problems. The synergy of classical numerical methods with modern AI is a promising area that could yield solvers with both the robustness of global methods and the efficiency of local high-order methods.

## 8. Conclusion and Future Work

**Conclusion:** In this work, we provided a comprehensive analysis of iterative methods for solving nonlinear equations, examining both theoretical foundations and practical performance. We reviewed classical methods (bisection, fixed-point iteration, Newton-Raphson, Secant) and modern high-order methods, discussing their convergence properties and

limitations. The theoretical part established definitions of convergence order, criteria for stability (e.g., contraction conditions, Kantorovich's theorem for Newton's method), and the concept of efficiency balancing convergence speed with computational cost. We highlighted that Newton's method is quadratically convergent and often optimal in efficiency for single equations, while Secant offers a no-derivative alternative with super linear convergence, and bracketing methods like Bisection guarantee convergence at the expense of speed. We also discussed how higher-order methods push the convergence order further, although they obey the Kung-Traub bound  $2^d - 1$  for  $d$  function evaluations per step, and introduced the efficiency index to compare methods on an equal footing. In the optimization strategies, we surveyed techniques like Anderson acceleration (which can dramatically speed up fixed-point iterations), damping and line searches (to ensure global convergence for Newton-type methods), hybrid algorithms (Brent's method combining secant and bisection), and emerging AI-based enhancements (learning-based meta-solvers that adapt iterative methods using machine learning).

The practical part of our study involved implementing Newton, Secant, and Bisection methods in Python and testing them on example equations. The results validated the theoretical expectations: Newton's method converged in just a few iterations (e.g. 4–6) to high accuracy, Secant needed slightly more (6–10 iterations), and Bisection was much slower (25+ iterations for similar accuracy), confirming quadratic vs. linear convergence in action. We also saw that Newton's speed comes with a caveat: it requires a sufficiently good starting guess and can diverge outside its convergence radius. Secant was more forgiving, especially when the initial points bracketed the root, and Bisection was unconditionally convergent given a bracket. These observations are in line with other research – for instance, Azure (2023) found Newton-Raphson to be “more efficient and reliable” than Secant on tested problems, which our experiments support (Newton converged with fewer iterations and was robust in those cases). We illustrated how in practical computing, one often uses a *combination* of methods: e.g., a few bisection steps to secure the root in an interval, then Newton to polish it off, which leverages the strengths of each approach.

**Contributions:** This study brings together a formal theoretical discussion and hands-on experimentation, giving a rounded perspective. The detailed citations to the literature provide an academic grounding – from classical convergence theorems and examples of new high-order methods, to modern improvements and uses in diverse fields. We demonstrated Python implementations of the algorithms and provided annotated results, which serve as a pedagogical example and could be a starting point for further experimentation or teaching. By spanning both theory and practice, the work shows not just *which* method is better, but *why* (through convergence analysis) and *in what context* (through examples and applications). One noteworthy insight is the importance of tailoring the solver to the problem: there is no one-size-fits-all iterative method – the choice depends on factors like availability of derivatives, desired precision, the behavior of the function, and whether reliability or speed is the priority.

**Limitations:** While our study was broad, it has certain limitations. Due to space, we focused on single-variable equations in the practical part; systems of nonlinear equations (multivariate root-finding) were discussed mostly qualitatively. The behavior in higher dimensions can differ – e.g., Newton's method might require good preconditioning or might converge to saddle points in optimization contexts, etc. We also did not implement more advanced methods like Anderson acceleration or hybrid algorithms in code (we discussed them conceptually). A

hands-on comparison of, say, Newton vs. Broyden vs. Anderson on a system of equations would further illuminate performance trade-offs, but that was beyond our scope here. Additionally, our AI-enhanced methods discussion was exploratory; we did not develop a new machine learning model for root-finding but rather reviewed existing ideas. The integration of AI with numerical solvers remains an open-ended topic.

In conclusion, solving nonlinear equations iteratively remains a critical and active area of numerical analysis. The combination of deep theoretical understanding and modern computational techniques continues to produce more robust and faster algorithms. Our study reinforces fundamental knowledge and opens the door to these future explorations, aiming ultimately for solvers that are fast, reliable, and adaptive across the broad spectrum of nonlinear problems encountered in science and engineering.

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## Appendix

The code implementation (plots 1,3 and 4):

```
import math
import matplotlib.pyplot as plt
import numpy as np

# Define the function f(x) = cos(x) - x and its derivative f'(x)
def f(x):
    return math.cos(x) - x

def df(x):
    return -math.sin(x) - 1

# Newton-Raphson method implementation with iterate recording
def newton_method(f, df, x0, tol=1e-8, max_iter=100):
    x_values = [x0]
    for i in range(max_iter):
        fx = f(x_values[-1])
        if abs(fx) < tol:
            break
        dfx = df(x_values[-1])
        # Avoid division by zero
        if dfx == 0:
            print("Zero derivative encountered in Newton's method.")
            break
        x_new = x_values[-1] - fx/dfx
        x_values.append(x_new)
    return x_values

# Secant method implementation with iterate recording
def secant_method(f, x0, x1, tol=1e-8, max_iter=100):
    x_values = [x0, x1]
    for i in range(2, max_iter):
        f0 = f(x_values[-2])
        f1 = f(x_values[-1])
        if abs(f1) < tol:
            break
        if f1 - f0 == 0:
            print("Division by zero in Secant method.")
            break
        x_new = x_values[-1] - f1 * (x_values[-1] - x_values[-2]) / (f1 - f0)
        x_values.append(x_new)
    return x_values

# Bisection method implementation with iterate recording
def bisection_method(f, a, b, tol=1e-8, max_iter=100):
    x_values = []
```

Code Implementation (plots 2,5)

```
import numpy as np
import matplotlib.pyplot as plt

# -----
# Iterative Method Definitions
# -----
def newton_method(f, df, x0, tol=1e-8, max_iter=100):
    """Newton-Raphson method.
    Returns list of approximations, list of |f(x)| errors,
    count of f evaluations and count of derivative evaluations.
    """
    x = x0
    xs = [x0]
    errors = []
    f_evals = 0
    df_evals = 0
    for _ in range(max_iter):
        fx = f(x)
        f_evals += 1
        if abs(fx) < tol:
            break
        dfx = df(x)
        df_evals += 1
        if dfx == 0:
            print("Zero derivative encountered; stopping iteration.")
            break
        x = x - fx/dfx
        xs.append(x)
        errors.append(abs(f(x)))
    return xs, errors, f_evals, df_evals

def secant_method(f, x0, x1, tol=1e-8, max_iter=100):
    """Secant method.
    Returns list of approximations, list of |f(x)| errors, and count of f
    evaluations.
    """
    xs = [x0, x1]
    errors = []
    f_evals = 0
    for _ in range(max_iter):
        fx0 = f(xs[-2])
        fx1 = f(xs[-1])
        f_evals += 2
        if abs(fx1) < tol:
            break
```